

The Skewes number for twin primes: counting sign changes of $\pi_2(x) - C_2\text{Li}_2(x)$

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Abstract

The results of the computer investigation of the sign changes of the difference between the number of twin primes $\pi_2(x)$ and the Hardy–Littlewood conjecture $C_2\text{Li}_2(x)$ are reported. It turns out that $d_2(x) = \pi_2(x) - C_2\text{Li}_2(x)$ changes the sign at unexpectedly low values of x and for $x < 2^{48} = 2.81 \dots \times 10^{14}$ there are 477118 sign changes of this difference. It is conjectured that the number of sign changes of $d_2(x)$ for $x \in (1, T)$ is given by $\sqrt{T}/\log(T)$. The running logarithmic densities of the sets for which $d_2(x) > 0$ and $d_2(x) < 0$ are plotted for x up to 2^{48} .

Keywords: Primes, twins, Skewes number

Let $\pi(x)$ be the number of primes smaller than x and let $\text{Li}(x)$ denote the logarithmic integral:

$$\text{Li}(x) = \int_2^x \frac{du}{\log(u)}. \quad (1)$$

The Prime Number Theorem tells us that $\text{Li}(x)/\pi(x)$ tends to 1 for $x \rightarrow \infty$ and the available data (see [24, Table 14, p. 175] or [8, Table 5 and 6]) show that always $\text{Li}(x) > \pi(x)$. This last experimental observation was the reason for the common belief in the past, that the inequality $\text{Li}(x) > \pi(x)$ is generally valid. However, in 1914 J.E. Littlewood has shown [20] (see also [7]) that the difference between the number of primes smaller than x and the logarithmic integral up to x changes the sign infinitely many times. The smallest value x_S such that for the first time $\pi(x_S) \geq \text{Li}(x_S)$ holds is called Skewes number. We have used “ \geq ” to avoid the case of integer value of $\text{Li}(x_S)$, although we believe that for $n \in \mathbb{N}$ there will be $\text{Li}(n) \notin \mathbb{N}$, like we know $\log(n)$ is for $\forall n$ irrational. In 1933 S. Skewes [29] assuming the truth of the Riemann hypothesis argued that it is certain that $d(x) := \pi(x) - \text{Li}(x)$ changes sign for some $x_S < 10^{10^{34}}$. In 1955 Skewes [30] has found, without assuming the Riemann hypotheses, that $d(x)$ changes sign at some

$$x_S < \exp \exp \exp \exp(7.705) < 10^{10^{10^3}}.$$

This enormous bound for x_S was reduced by Cohen and Mayhew [5] to $x_S < 10^{10^{529.7}}$ without using the Riemann hypothesis. In 1966 Lehman [19] has shown that between 1.53×10^{1165} and 1.65×10^{1165} there are more than 10^{500} successive integers x for which $\pi(x) > \text{Li}(x)$. Following the method of Lehman in 1987 H.J.J. te Riele [31] has shown that between 6.62×10^{370} and 6.69×10^{370} there are more than 10^{180} successive integers x for which $d(x) > 0$. The lowest present day known estimation of the Skewes number is around 10^{316} , see [2] and [27].

The number of sign changes of the difference $d(x)$ for x in a given interval $(1, T)$, which is commonly denoted by $\nu(T)$, see [7], was discussed for the first time by A.E. Ingham in 1935 [12] chapter V, [11] and next by S. Knapowski [16]. Regarding the number of sign changes of $d(x)$ in the interval $(1, T)$, Knapowski [16] proved that

$$\nu(T) \geq e^{-35} \log \log \log \log T \quad (2)$$

provided $T \geq \exp \exp \exp \exp(35)$. Further results about $\nu(T)$ were obtained by J. Pintz [21], [22] and J. Kaczorowski [13], [14]. In particular, in [14] Kaczorowski proved that there exists such a positive constant c_3 that for sufficiently large T the inequality

$$\nu(T) \geq c_3 \log(T) \quad (3)$$

holds. In [28] J.-C. Schlage-Puchta proved, assuming the Riemann Hypothesis, that

$$\nu(T) > \frac{\log(T)}{e^{16.7}} - 1. \quad (4)$$

More general results on the sign changes can be found in the recent paper [15].

In this paper we will look for the analog of the Skewes number for the twin primes, i.e. pairs of primes separated by 2: $\{(3,5), (5,7), (11,13), \dots, (59, 61), \dots\}$.

Let us denote the number of twin primes pairs $(p, p+2)$ with $p+2 < x$ by $\pi_2(x)$. Then the unproved (see however [25]) conjecture B of Hardy and Littlewood [9] on the number of prime pairs $p, p+d$ applied to the case $d=2$ gives, that

$$\pi_2(x) \sim C_2 \text{Li}_2(x) \equiv C_2 \int_2^x \frac{u}{\log^2(u)} du, \quad (5)$$

where C_2 is called “twin constant” and is defined by the following infinite product:

$$C_2 \equiv 2 \prod_{p>2} \left(1 - \frac{1}{(p-1)^2}\right) = 1.3203236316937\dots \quad (6)$$

For the first time the conjecture (5) was checked computationally up to 8×10^{10} by R. P. Brent [4] who noticed the sign changes of the difference $\pi_2(x) - C_2 \text{Li}_2(x)$, but he did not mention neither the analogy with Skewes number nor did not count these sign changes. We analyzed the difference $d_2(x) := \pi_2(x) - C_2 \text{Li}_2(x)$ using the computer for x up to $T = 2^{48} \approx 2.814 \times 10^{14}$. It took 195 CPU days to reach $T = 2^{48}$ on the 64 bits AMD[®] Opteron 2700 MHz processor.

To calculate the integral $\text{Li}_2(x)$ during the main run of the program till 2^{48} we have used the 10-point Gauss quadrature [23]. This integral was calculated numerically in successive intervals between consecutive twins and added to the previous value. Such a method is not very time consuming and the number of performed arithmetical operations does not depend on x . There are also power series representations of the logarithmic

integral. We use the following convention for the $\text{li}(x)$ (here *v.p.* stands for French *valeur principale* i.e. Cauchy principal value):

$$\text{li}(x) = v.p. \int_0^x \frac{du}{\log(u)} \equiv \lim_{\epsilon \rightarrow 0} \left(\int_0^{1-\epsilon} \frac{du}{\log(u)} + \int_{1+\epsilon}^x \frac{du}{\log(u)} \right), \quad (7)$$

hence we have $\text{Li}(x) = \text{li}(x) - \text{li}(2)$. Integration by parts gives the asymptotic expansion:

$$\text{li}(x) \sim \frac{x}{\log(x)} + \frac{x}{\log^2(x)} + \frac{2x}{\log^3(x)} + \frac{6x}{\log^4(x)} + \cdots + \frac{n!x}{\log^{n+1}(x)} + \cdots \quad (8)$$

which should be cut at $n_0 = \lfloor \log(x) \rfloor$ — beginning with this index the following terms are increasing. There is a series giving $\text{li}(x)$ for all $x > 1$ and quickly convergent which has $n!$ in denominator and $\log^n(x)$ in nominator instead of opposite order in (8) (see [3, p.126, Entry 14])

$$\int_{\mu}^x \frac{du}{\log(u)} = \gamma + \log \log(x) + \sum_{n=1}^{\infty} \frac{\log^n(x)}{n \cdot n!} \quad \text{for } x > 1, \quad (9)$$

where $\gamma = 0.5772156649\dots$ is the Euler-Mascheroni constant and $\mu = 1.451369234883381\dots$ is the Soldner constant defined by (see [3, p.123, eq.(11.3)])

$$\text{li}(\mu) = v.p. \int_0^{\mu} \frac{du}{\log(u)} = 0.$$

Even faster converging series was discovered by Ramanujan [3, p.130, Entry 16]:

$$\int_{\mu}^x \frac{du}{\log(u)} = \gamma + \log(\log(x)) + \sqrt{x} \sum_{n=1}^{\infty} \frac{(-1)^{n-1} (\log(x))^n}{n! 2^{n-1}} \sum_{k=0}^{\lfloor (n-1)/2 \rfloor} \frac{1}{2k+1} \quad \text{for } x > 1. \quad (10)$$

Because we have

$$\text{Li}_2(x) = \text{Li}(x) - \frac{x}{\log(x)}$$

it is possible to calculate values of $\text{Li}_2(x)$ using the above series. Disadvantage of these series is that the number of operations (including time consuming calculation of $\log(x)$) increases with x and is larger than number of operations needed in the numerical integration.

As for the set of all primes initially the inequality $C_2 \text{Li}_2(x) > \pi_2(x)$ holds, but it turns out that there are surprisingly many sign changes of $d_2(x) = \pi_2(x) - C_2 \text{Li}_2(x)$ for x in the interval $(1, 2^{48})$. The first sign change of $d_2(x)$ appears at the twin pair (1369391,

1369393) and up to $T = 2^{48}$ there are 477118 sign changes of $d_2(x)$. We have collected positions of all these sign changes in one file which is available for downloading from http://www.ift.uni.wroc.pl/~mwolf/Skewesy_twins.zip. Let $\nu_2(T)$ denote, by analogy with usual primes, the number of sign changes of $d_2(x)$ in the interval $(1, T)$. The Table I contains the recorded number of sign changes of $\pi_2(x) - C_2\text{Li}_2(x)$ up to $T = 2^{21}, 2^{22}, \dots, 2^{48}$. We have checked the numbers $\nu_2(T)$ up to $T = 2^{34} = 1.718 \times 10^{10}$ independently calculating the integral $\text{Li}_2(x)$ from the series (10) and these results are presented in Table I in the third column and are marked with asterisk. The first 1274 positions of sign

TABLE I

The number of sign changes of $d_2(x)$

T	$\nu_2(T)$	$\nu_2(T)(*)$	$\sqrt{T}/\log(T)$	T	$\nu_2(T)$	$\sqrt{T}/\log(T)$
2^{21}	29	29	99	2^{35}	12682	7641
2^{22}	29	29	134	2^{36}	23634	10505
2^{23}	29	29	182	2^{37}	31641	14455
2^{24}	29	29	246	2^{38}	31641	19905
2^{25}	29	29	334	2^{39}	31641	27428
2^{26}	238	238	455	2^{40}	38899	37819
2^{27}	854	854	619	2^{41}	55106	52180
2^{28}	1226	1226	844	2^{42}	90355	72037
2^{29}	1226	1226	1153	2^{43}	161031	99506
2^{30}	1226	1226	1576	2^{44}	161031	137525
2^{31}	1226	1226	2157	2^{45}	161031	190168
2^{32}	2854	2852	2955	2^{46}	405289	263091
2^{33}	7383	7381	4052	2^{47}	472000	364151
2^{34}	9115	9113	5562	2^{48}	477118	504258

changes of $d_2(x)$ obtained by these two methods of calculating the integral $\text{Li}_2(x)$ were the same. The first difference between both methods appears at twin pairs (3067608611, 3067608613) and (3067609091, 3067609093), which were not detected using the more

accurate formula (10). Next twin primes detected by the two methods are the same until the twin pairs (7809444029, 7809444031). In general, among over 9100 sign changes up to 2^{34} there were 17 differences in the positions of sign changes of $d_2(x)$ obtained by two methods of calculating the integral $\text{Li}_2(x)$.

The values of T searched by the direct checking are of small magnitude from the point of view of mathematics, but large for modern computers.

The observed numbers $\nu_2(T)$ behave somewhat erratically, see Fig.1, in particular there are large gaps without any change of sign of the $d_2(x)$. If one assumes the power-like dependence of $\nu_2(T)$ then the fit by the least square method gives the function aT^b , where $a = 0.2723\dots$ and $b = 0.4389\dots$. Instead of such accidentally looking parameters of the pure power-like dependence we suggest the function $\sqrt{T}/\log(T)$ as an approximation to $\nu_2(T)$ — it is a more natural function, without any free parameters and taking values very close to the least square fit aT^b , see Figure 1. Thus we state the following conjecture:

$$\nu_2(T) \sim \sqrt{T}/\log(T) . \quad (11)$$

We have picked out function $\sqrt{T}/\log(T)$ after a few trials and we are not able to give even heuristic arguments in favour of it. The conjecture (11) is supported by the fact that there are 10 crossings of the curve $\sqrt{T}/\log(T)$ with the staircase-like plot of $\nu_2(T)$ obtained directly from the computer data. The last column in the Table 1 contains the values of the function $\sqrt{T}/\log(T)$. If the conjecture (11) is true, then there is infinity of twins.

It seems to be very difficult to gain some analytical insight to why there are so many sign changes of $\pi_2(x) - C_2\text{Li}_2(x)$. As (5) is not proved, hence error term for it is also not known (for heuristic approximate formula for averages of the remainders in the Hardy–Littlewood conjecture B see [18]). The best error term for Prime Number Theorem under the Riemann Hypothesis is $|\pi(x) - \text{Li}(x)| = \mathcal{O}(\sqrt{x}\log(x))$. In the Fig.2 we present the computer data for two functions: the running difference $d(x) = \text{Li}(x) - \pi(x)$ and the error term:

$$\Delta(x) = \max_{2 < t < x} |\pi(t) - \text{Li}(t)| , \quad (12)$$

Characteristic oscillations of $d(x)$ are fully described by the explicit formula for $\pi(x)$, see

e.g. [8, formula (3) and Figure 4]. In the Fig. 3 $|d_2(x)|$ and the error term

$$\Delta_2(x) = \max_{2 < t < x} |\pi_2(t) - C_2 \text{Li}_2(t)| \quad (13)$$

is plotted for $x < 2^{48}$. As it is seen from these figures the behavior of $d(x)$ and $d_2(x)$ is completely different with rapid oscillations of $d_2(x)$ of many orders. However the functions $\Delta(x)$ and $\Delta_2(x)$ are quite similar: the error term for twins $\Delta_2(x)$ is smaller than $\Delta(x)$ but the difference is not significant: the power-like fits to $\Delta(x)$ and $\Delta_2(x)$ give:

$$\alpha x^\beta, \quad \alpha = 0.209 \dots, \quad \beta = 0.45 \dots \quad \text{for } \Delta(x) \quad (14)$$

$$\alpha_2 x^{\beta_2}, \quad \alpha_2 = 0.337 \dots, \quad \beta_2 = 0.418 \dots \quad \text{for } \Delta_2(x). \quad (15)$$

Here the slopes $\beta \approx \beta_2$ and prefactors α and α_2 are very close. Thus it seems that the sizes of the error terms do not account for enormous difference in the value of Skewes number. In fact all considerations of Skewes, Kaczorowski and others were based on existence of explicit formulas and there are no analogs of explicit formulas for twins. However Turan [33] introduced the following Dirichlet series with the aim to study twins:

$$T(s) := \sum_{n>3} \frac{\Lambda(n-1)\Lambda(n+1)}{n^s} \quad (\Re s > 1), \quad (16)$$

where $\Lambda(n)$ is the von Mangoldt function:

$$\Lambda(n) = \begin{cases} 0 & \text{if } n = 1 \\ \log p & \text{if } n = p^k \text{ for some prime } p \text{ and integer } k \geq 1, \\ 0 & \text{if } n \text{ has at least two different prime factors.} \end{cases} \quad (17)$$

In 2004, in a preprint publication [1] Arenstorf attempted to prove that there are infinitely many twins. Arenstorf tried to continue analytically $T(s) - C_2/(s-1)$ to $\Re s = 1$, but shortly after an error in the proof was pointed out by Tenenbaum [32]. For recent progress in the direction of the proof of the infinite number of twins see [17].

The comparison of Figures 2 and 3 shows, that $\pi_2(x) \sim C_2 \text{Li}_2(x)$ is better than $\pi(x) \sim \text{Li}(x)$ in the sense that there are almost half a million points where $d_2(x)$ is zero in the Fig.3 while in the Fig. 2 there are no crossings of x axis at all. This observation can be quantifying with the notion of the logarithmic density. In [26] it was proposed to

use the logarithmic density to measure the different biases in the distribution of prime numbers. In particular, for the case of the sign changes of $d(x)$ it was shown that the logarithmic density of the set $\{x : \text{Li}(x) < \pi(x)\}$ defined by

$$\delta_{\{x:\text{Li}(x)<\pi(x)\}} = \lim_{x \rightarrow \infty} \frac{1}{\log(x)} \sum_{\substack{2 \leq n < x \\ \text{Li}(n) < \pi(n)}} \frac{1}{n} \quad (18)$$

is equal to $\delta_{\{x:\text{Li}(x)<\pi(x)\}} = 2.7 \dots \times 10^{-7}$. Hence in some precisely defined sense the inequality $\text{Li}(x) > \pi(x)$ holds almost everywhere. Here we will define two logarithmic densities for twin primes as follows:

$$\delta_+ = \lim_{x \rightarrow \infty} \frac{1}{\log(x)} \sum_{\substack{2 \leq n < x \\ d_2(n) > 0}} \frac{1}{n} \quad (19)$$

$$\delta_- = \lim_{x \rightarrow \infty} \frac{1}{\log(x)} \sum_{\substack{2 \leq n < x \\ d_2(n) < 0}} \frac{1}{n}. \quad (20)$$

We do not have at our disposal any formulas like those in [26] and we have to turn to the brute force numerical calculation of finite size approximations $\delta_+(x)$ and $\delta_-(x)$ given by expressions (19) and (20) without limit operation $\lim_{x \rightarrow \infty}$. In these computation we have used positions of all sign changes collected earlier. The resulting running logarithmic densities are plotted in Figure 4. The sum for $\delta_-(x)$ starts from $1/5$, because 5 is the end of the first twin primes pair. It is a reason why the plot of $\delta_-(x)$ in Fig.4 starts from about 0.67. Up to $x = 2^{31}$ the data for Figure 4 was obtained by direct summing of the harmonic sums, for $x > 2^{31} \approx 2.15 \times 10^9$ the incredible accurate approximation [6], [10, pp. 76-78]:

$$\sum_{k=n}^m \frac{1}{k} = \log \left(m + \frac{1}{2} \right) - \log \left(n - \frac{1}{2} \right) + \mathcal{O} \left(\frac{1}{n^2} \right) \quad (21)$$

was used (the implied in \mathcal{O} constant is much smaller than 1). For $n \approx 10^9$ the error made by using the above formula is of the order 10^{-18} . To calculate the harmonic series up to $x = 2.8 \times 10^{14}$ directly by adding all numbers $1/n$ would take from one to a few months of CPU time, depending on the processor. The plots presented in Fig.4 suggest following the conjecture

$$\delta_+ = \delta_- = \frac{1}{2}. \quad (22)$$

The difference of many hundreds of orders between values of x such that $\pi(x) - \text{Li}(x)$ and $\pi_2(x) - C_2\text{Li}_2(x)$ changes the sign for the first time is astonishing. We can give an example from physics. Let us make the mapping: sign changes of $d(x)$ correspond to energy levels of hydrogen and sign changes of $d_2(x)$ correspond to the spectrum of helium. Then ground states of hydrogen and of helium will correspond to x_S and first sign change of $d_2(x)$ accordingly. The experiments show that the energies of the ground states of the hydrogen and helium are -13.6 eV and -79 eV respectively and do not differ by hundreds of orders!

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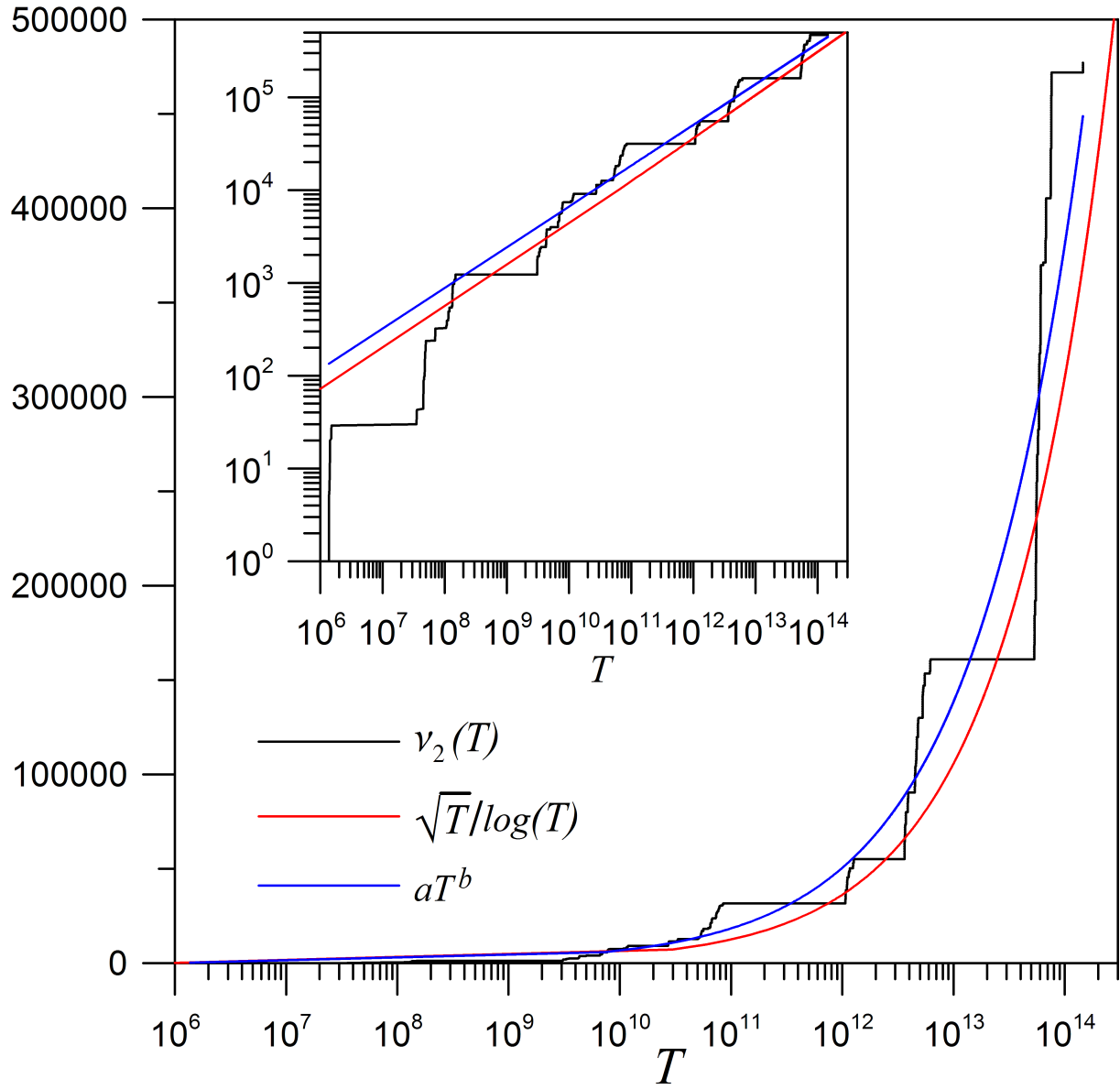


Fig.1 The plot showing the comparison of the actual values of $\nu_2(T)$ found by a computer search with the conjecture (11). There are 10 crossing of the function $\nu_2(T)$ and $\sqrt{T}/\log(T)$ in this plot up to 2^{48} . All 477118 sign changes of $d_2(x)$ are plotted. In the inset plot on the double logarithmic scale is presented.

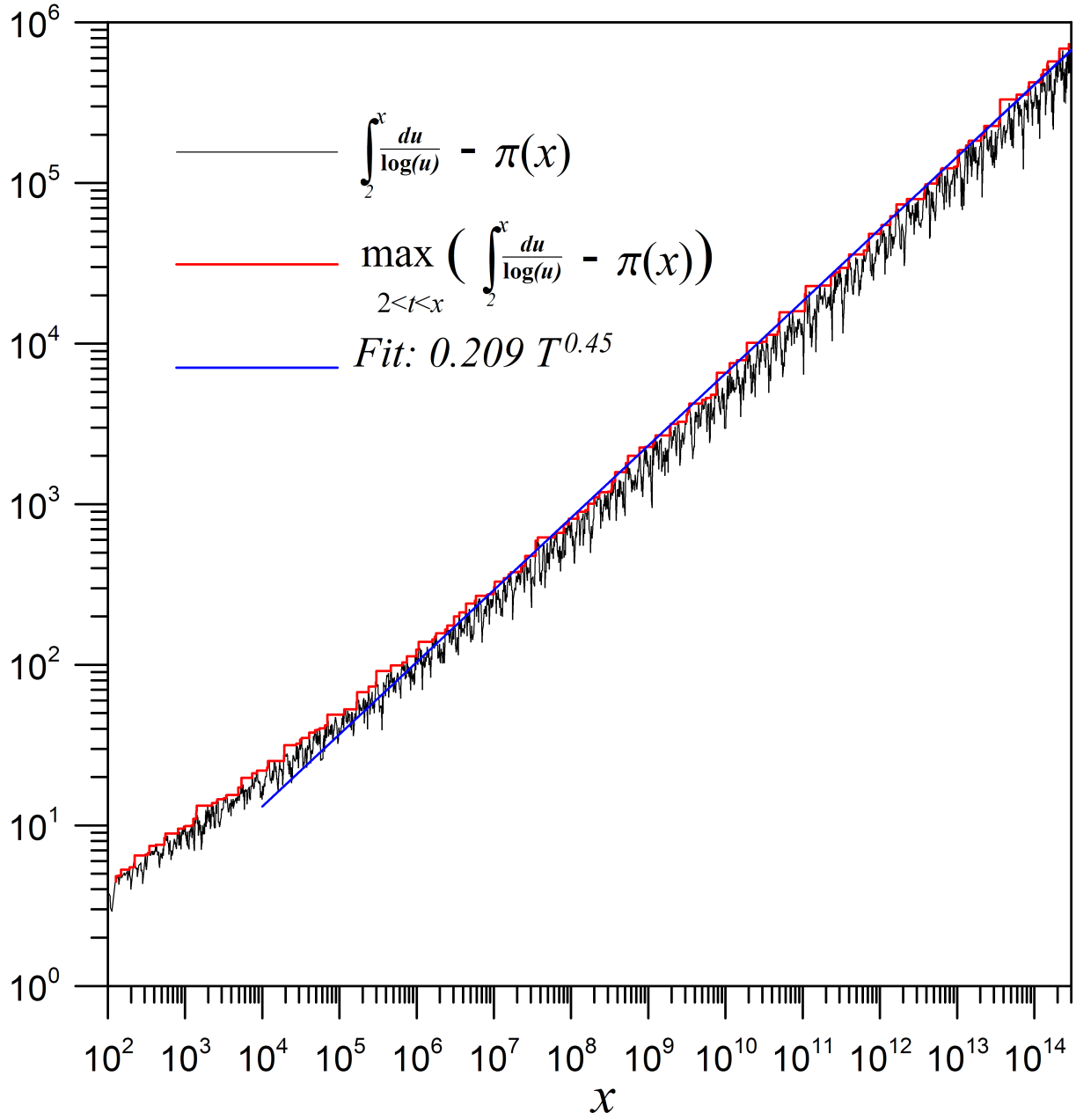


Fig.2 The plot of $d(x)$ and error term $\Delta(x)$. The power fit was made for $10^6 < x < 2^{48}$. The first crossing of the axis x will appear around 10^{316} .

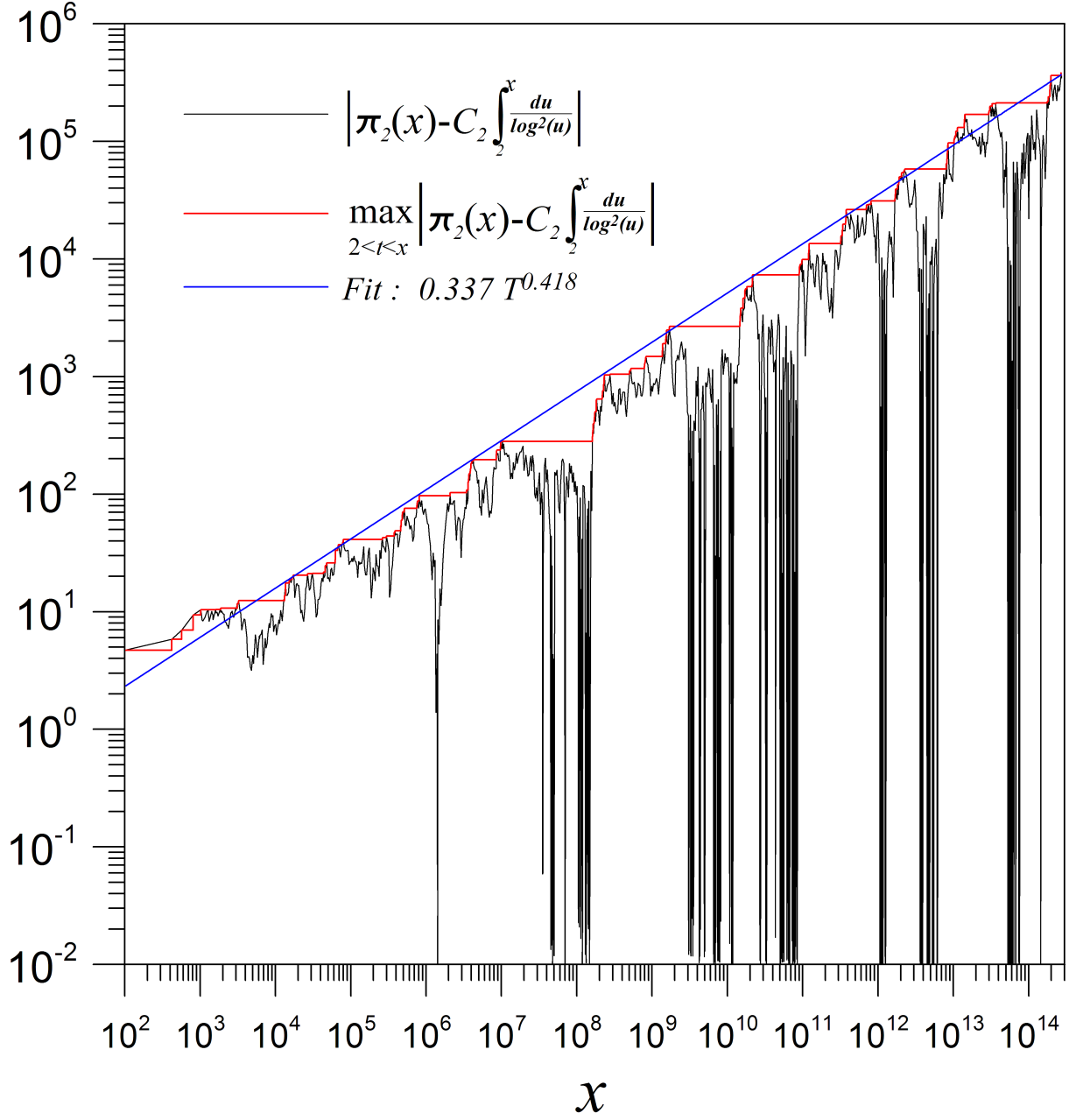


Fig.3 The plot of $|d_2(x)|$ and error term $\Delta_2(x)$. Sign changes of the $d_2(x)$ and values smaller than 10^{-2} were artificially set to 10^{-2} . In blue the power-like fit $0.337 \times x^{0.418}$ to $\Delta_2(x)$ obtained by the least-square method is plotted.

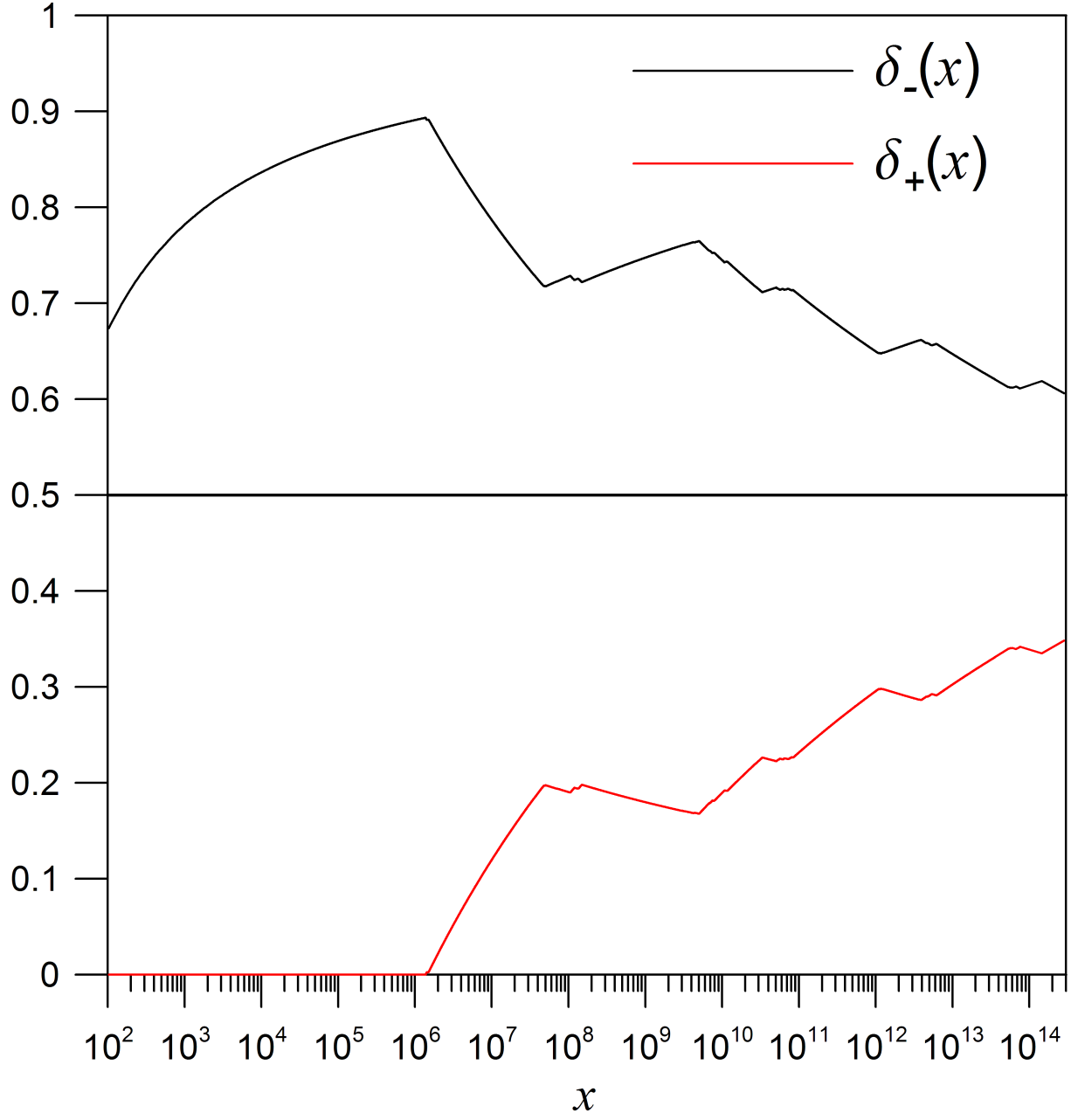


Fig.4 The plots of the running logarithmic densities $\delta_+(x), \delta_-(x)$ defined in the text. Each plot consists of 28025 points: the values of $\delta(x)$'s were recorded at the progression $x = 100 \times (1.001)^n$.